FOURIER-TRANSFORM MICROWAVE AND MILLIMETERWAVE SPECTROSCOPY OF CH_2IBr IN ITS GROUND VIBRATIONAL STATE

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Halo-substituted methanes constitute a class of molecules that are important in various fields, from spectroscopy to quantum-chemical calculations. They are also gaining interest due to their potential adverse impact on the atmospheric chemistry.[a]

In the series of the CH_2IX iodomethanes where X = {F, Cl, Br}, only the rotational spectra of CH_2IF [b] and CH_2ICl [c] have been published. We present our investigations on the high-resolution rotational spectroscopy of the two bromine isotopologues of bromoiodomethane, $CH_2I^{79}Br$ and $CH_2I^{81}Br$.

Due to the lack of spectroscopic information available for this compound, high-level quantum-chemical calculations were essential to guide the microwave and millimeterwave spectral assignments of both μ_a- and μ_b-type transitions. They provided rotational and centrifugal distortion constants (quartic and sextic), as well as the quadrupole-coupling tensor of the iodine ($I_I = 5/2$) and bromine ($I_{Br} = 3/2$) nuclei.

More than 1900 lines have been analyzed, leading to an accurate determination of molecular constants for both isotopologues. The experimental structure (r_0) of the title species has been derived from the two sets of rotational constants.

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